

On the symplectic integration of the Klein Gordon lattice model

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ABSTRACT. We investigate the performance of various methods of symplectic integration, which are based on two part splitting of the integration operator, for the numerical integration of multidimensional Hamiltonian systems. We implement these schemes to study the behaviour of the one-dimensional quartic Klein Gordon disordered lattice with many degrees of freedom (of the order of a few hundreds) and compare their efficiency for the weak chaos regime of the system's dynamics. For this reason we perform extensive numerical simulations for each considered integration scheme. In this process, the second moment and the participation number of propagating wave packets, along with the system's relative energy error and the required CPU time are registered and compared.

Keywords: symplectic integration, Klein-Gordon lattice, disordered systems, Hamiltonian systems

1. Introduction

Symplectic integrators (SIs) are known to preserve the symplectic nature of the Hamiltonian system and keep bounded the error of the computed value of the Hamiltonian. This is one of the advantages that these integrators have over general purpose integrators. In ([2],[21],[4]) various SIs have been applied in the study of the chaotic behavior of two one-dimension Hamiltonian lattices, namely the Klein-Gordon (KG) chain and the Discrete NonLinear Schrödinger model. These studies showed that there exist different dynamical behaviors, namely the so called weak chaos, strong chaos and the self trapping regime. In this study we consider a wider range of SIs for integration of multidimensional Hamiltonian systems.

In the next section we give a brief discussion of the KG lattice as the Hamiltonian model to use in this study. We also give a description of SIs of generalised order, order two and order four with an insight of how composition techniques are used to generate schemes of higher order. Section 3 is devoted to comparing the performance of these SIs for the integration of the KG lattice after which we present our conclusions in section 4.

2. The KG Hamiltonian model and the integration schemes

The Hamiltonian H of the one-dimensional KG lattice model of coupled anharmonic oscillators with N degrees of freedom is

$$H(\mathbf{q}, \mathbf{p}) = \sum_i \frac{p_i^2}{2} + \frac{\epsilon_i}{2} q_i^2 + \frac{1}{4} q_i^4 + \frac{1}{2W} (q_{i+1} - q_i)^2, \quad (0.1)$$

where q_i and p_i are the generalised position and momenta of site i respectively. ϵ_i are potential strengths that are chosen uniformly from the interval $[\frac{1}{2}, \frac{3}{2}]$, and W is a parameter that determines the extent of disorder in the lattice. From (0.1), the resulting equations of motion

$$\frac{dq_i}{dt} = p_i, \quad \frac{dp_i}{dt} = -\epsilon_i q_i - q_i^3 + \frac{1}{W} (q_{i+1} + q_{i-1} - 2q_i) \quad (0.2)$$

can be written as $\frac{d\mathbf{z}}{dt} = \{\mathbf{z}, H\} =: L_H \mathbf{z}$, where $\mathbf{z} = (\mathbf{q}, \mathbf{p})$, L_H is the so called Poisson bracket that is defined by $\{F, G\} := \sum_i \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right)$, for differentiable functions $F(\mathbf{z})$ and $G(\mathbf{z})$. Using initial conditions $\mathbf{z}_0 = \mathbf{z}(0)$, we therefore get a formal solution

$$\mathbf{z}(t) = \sum_{i \geq 0} \frac{t^i}{i!} L_H^i \mathbf{z}_0 = e^{tL_H} \mathbf{z}_0.$$

The Hamiltonian (0.1) can be split into two integrable parts as $H(\mathbf{z}) = A(\mathbf{p}) + B(\mathbf{q})$ where

$$A = \sum_i \frac{p_i^2}{2}, \quad B = \sum_i \frac{\epsilon_i}{2} q_i^2 + \frac{1}{4} q_i^4 + \frac{1}{2W} (q_{i+1} - q_i)^2 \quad (0.3)$$

and the action of the operators $e^{\tau L_A}$ and $e^{\tau L_B}$ is known analytically.

A SI approximates the operator $e^{\tau L_H}$ by a product of operators $e^{a_i \tau L_A}$ and $e^{b_i \tau L_B}$ where the constants a_i and b_i are chosen depending on the required order of the SI [14].

In our study we consider the performance of order two, order four and generalised order SIs $ABA82$, $ABA864$, $ABAH864$ of [22] in integrating system (0.1).

The order two SIs $SABA_2$ and $SBAB_2$ [3, 5] are

$$SABA_2 = e^{c_1 \tau L_A} e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} e^{c_1 \tau L_A}$$

where $c_1 = \frac{1}{2} - \frac{1}{2\sqrt{3}}$, $c_2 = \frac{1}{\sqrt{3}}$, $d_1 = \frac{1}{2}$, and

$$SBAB_2 = e^{c_1 \tau L_B} e^{d_1 \tau L_A} e^{c_2 \tau L_B} e^{d_1 \tau L_A} e^{c_1 \tau L_B}$$

where $d_1 = \frac{1}{2}$, $c_1 = \frac{1}{6}$ and $c_2 = \frac{2}{3}$

The order of the SIs $SABA_2$ and $SBAB_2$ can be improved to order four by including a corrector term

$$\mathbf{C} = e^{-\tau^3 \epsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}}$$

where the value of c is $\frac{(2-\sqrt{3})}{24}$ for $SABA_2$ and $\frac{1}{72}$ for $SBAB_2$. We therefore get the so called $SABA_2$ with corrector, $SABA_2 wc = \mathbf{C} SABA_2 \mathbf{C}$ and $SBAB_2$ with corrector $SBAB_2 wc = \mathbf{C} SBAB_2 \mathbf{C}$

We also consider SIs of generalised order (8, 2) and (8, 6, 4) [6, 12].

Order (8, 2) SI $ABA82$:

$$ABA82 = e^{a_1 \tau L_A} e^{b_1 \tau L_B} e^{a_2 \tau L_A} e^{b_2 \tau L_B} e^{a_3 \tau L_A} e^{b_2 \tau L_B} e^{a_2 \tau L_A} e^{b_1 \tau L_B} e^{a_1 \tau L_A}$$

with the coefficients a_i , b_i stated in [22] and order (8, 6, 4) SIs $ABA864$ and $ABAH864$ as defined in [12] together with the corresponding coefficients.

For a symmetric order two integrator S_2 , an order four integrator $S_2 Y4$ was constructed in [7] by Yoshida using composition techniques. That is to say,

$$S_2 Y4(\tau) := S_2(a_1 \tau) S_2(a_0 \tau) S_2(a_1 \tau)$$

where

$a_0 = \frac{2^{\frac{1}{3}}}{2-2^{\frac{1}{3}}}$ and $a_1 = \frac{1}{2-2^{\frac{1}{3}}}$. In particular we study the behavior of order four SIs $SABA_2 Y4$ and $SBAB_2 Y4$

In [8], using the order two SI Leap-Frog (LF) an order four scheme $Sz4$ was constructed:

$$Sz4(\tau) = LF(k\mathbf{z}) LF((1-2k)\mathbf{z}) LF(p\mathbf{z})$$

where . It can be easily seen that when the Yoshida composition technique is applied to LF , one ends up with $Sz4$.

Forest and Ruth constructed a fourth order SI which we shall call $FRO4$ defined as

$$FRO4 = e^{a_1 \tau L_A} e^{b_1 \tau L_B} e^{a_2 \tau L_A} e^{b_2 \tau L_B} e^{a_3 \tau L_A} e^{b_3 \tau L_B} e^{a_4 \tau L_A} e^{b_3 \tau L_B} e^{a_3 \tau L_A} e^{b_2 \tau L_B} e^{a_2 \tau L_A} e^{b_1 \tau L_B} e^{a_1 \tau L_A}$$

with the coefficients a_i , b_i as specified in [9].

3. Numerical results

We consider a disorder realization of H in (0.1) for a total of 1000 sites with a random value of ϵ_i at site i . Fixing $W = 4$ and 0 initial displacement we make an initial excitation of the central site with a total energy of 0.4. We then keep track of the second moment $m2$, participation number P and CPU time.

The energy of site i at a time t is

$$h_i = \frac{p_i^2}{2} + \frac{\epsilon_i}{2} q_i^2 + \frac{1}{4} q_i^4 + \frac{1}{4W} (q_{i+1} - q_i)^2 \quad (0.4)$$

and $\bar{i} := \sum_i i \frac{h_i}{E_t}$.

With energy E_t at time t , a normalised energy distribution $\frac{h_i}{E_t}$ of site i , $m2 = \sum_i (i - \bar{i})^2 \frac{h_i}{E_t}$ is a measure of the rate at which the wave packet spreads from the initially excited central site to all sites in the lattice and $P = \frac{1}{\sum_i (\frac{h_i}{E_t})^2}$ quantifies the proportion of excited sites in the entire lattice.

In order to compare the performance of the different SIs, we adjust the time step τ so that the absolute relative energy error $REe := \left| \frac{E_t - E_0}{E_0} \right| \lesssim 10^{-5}$ at a time t of the evolution; where E_0 and E_t are the energies of the system at times 0 and t respectively. For each of the SIs we ensure that there is a global constistance amongst the SIs in the evolution of $m2$ and P for capturing the dynamics of the wave packet. For each of the SIs we then record the CPU time which is required to perform the simulations.

FIGURE 1 shows the results obtained when we integrate (0.2) using order two schemes $SBAB_2$ (red curve) and $SABA_2$ (green curve) and generalised order scheme $ABA82$ (gray curves). From this figure we see that with all the schemes portraying practically the same dynamical behavior of the wave packet with respect to $m2$ and P , $ABA82$ has the best performance since it requires the least CPU time compared to the other SIs.

In FIGURE 2 we have results for the integration of equations of motion 0.1 using order four schemes $SABA2wc$ (red curve), $Sz4$ (blue curve), $SBAB_2Y4$ (pink curve) and generalized order schemes $ABAH864$ (green curve) and $ABA82$ (gray curves). The generalised order scheme $ABA82$ requires the highest CPU time whereas the schemes $SABA2wc$ and $ABAH864$ show a better performance compared to other schemes since they require the least CPU time.

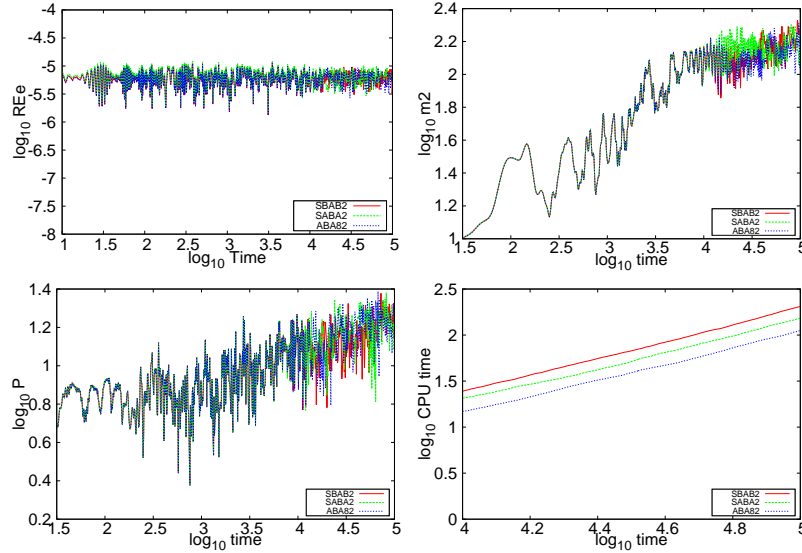


FIGURE 1. Results for the integration of (0.2), by the order two schemes $SBAB_2$ for $\tau = 0.016$ (red curve) and $SABA_2$ for $\tau = 0.0185$ (green curve) and $ABA82$ of generalised order (8, 2) for $\tau = 0.032$ (gray curves). The panels show the logarithms of the relative energy error, second moment, participation number and the CPU time required for evolution upto time 10^5 .

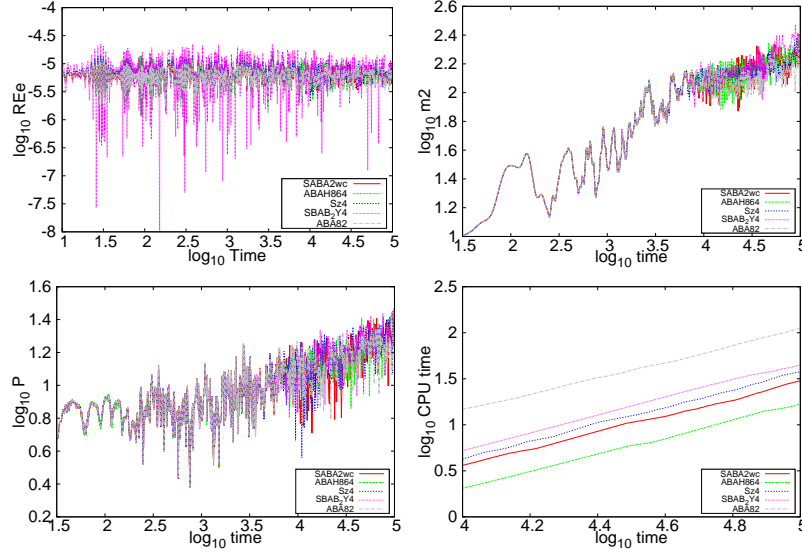


FIGURE 2. Results for the integration of (0.2), by the order four schemes $SABA2wc$ for $\tau = 0.165$ (red curve), $ABAH864$ for $\tau = 0.355$ (green curve), $Sz4$ for $\tau = 0.084$ (blue curve), $SBAB2Y4$ for $\tau = 0.13$ (pink curve) and $ABA82$ for $\tau = 0.032$ (gray curves). The panels show the logarithms of the relative energy error, second moment, participation number and the CPU time required for evolution upto time 10^5 .

In FIGURE 3 we have the results for the integration when we use $SABA2Y4$ (red curves), $SBAB2wc$ (green curve), $ABAH864$ (gray curve), $ABA864$ (pink curve) and $FRO4$ (light blue curves). The SIs of generalised order $ABAH864$ and $ABA864$ show a better performance compared to all the other SIs that have been used in the simulations. The SI $ABA864$ reveals the best performance in terms of least CPU time amongst all the SIs that were used in this work.

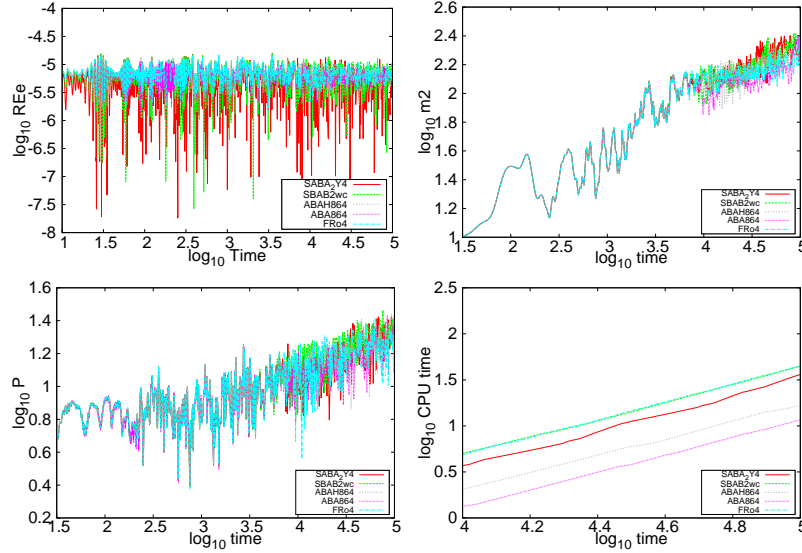


FIGURE 3. Results for the integration of (0.2), by the order four schemes $SABA2Y4$ for $\tau = 0.1255$ (red curves), $SBAB2wc$ for $\tau = 0.134$ (green curve), $ABAH864$ for $\tau = 0.355$ (gray curve), $ABA864$ for $\tau = 0.4855$ (pink curve) and $FRO4$ for $\tau = 0.084$ (light blue curves). The panels show the logarithms of the relative energy error, second moment, participation number and the CPU time required for evolution upto time 10^5 .

4. Summary and conclusions

In this work we have studied the integration of the Klein-Gordon lattice model for the so called weak chaos regime. We have used SIs of order two, four and or generalised order. The class of schemes of generalised order have proven to perform better compared to the other schemes that have been tested in this study. Of the three schemes of generalised order, *ABA864* performed better than *ABAH864* and *ABA82* in the integration of the KG model.

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REFERENCES

- [1] Ch. Skokos, E. Gerlach, J. D. Bodyfelt, G. Papamikos, S. Eggl, “High order three part split symplectic integrators: Efficient techniques for long time simulation of the disordered discrete nonlinear Schrodinger equation”, 2014 Phy Lett A 378 1809-18115
- [2] J. E. Chambers, “A hybrid symplectic integrator that permits close encounters between massive bodies”, Mon. Not. R. Astron. Soc. 304, 793-799 (199910).
- [3] D. O. Krimer, S. Flach, “Statistics of wave interactions in nonlinear disordered systems”, Phys. Rev. E 82, 046221 (2010).
- [4] S. Flach, D. O. Krimer and Ch. Skokos, Phy. Rev. Lett. 102, 024101 (2009).
- [5] J. Laskar and P. Robutel, “High order symplectic integrators for perturbed Hamiltonian systems”, Celestial Mechanics, vol. 80, pp. 39-62 (2001).
- [6] R. I. McLachlan, “Composition methods in the presence of small parameters”, BIT 35 (1995), 258-268.
- [7] H. Yoshida, “Construction of higher order symplectic integrators”, Phy. Lett. A, vol. 150, no. 5,6,7 (1990).
- [8] M. Suzuki, “General theory of fractal path integrals with applications to many-body theories and statistical physics”, J. Math. Phys. **32** (2), 1991.
- [9] E. Forest and R. D. Ruth, “Fourth-order symplectic integration”, Physica D 43 (1990) 105-117
- [10] L. Nadolski and J. Laskar, “Application of a new class of symplectic integrators to accelerator tracking”, EPAC02 2002, proceedings of the European Particle accelerator conference.
- [11] Ch. Skokos and Y. Papaphilippou, EPAC08 2008, proceedings of the European Particle accelerator conference.
- [12] S. Blanes, F. Casas, A. Farres, J. Laskar, J. Makazaga, A. Murua, “New families of symplectic splitting methods for numerical integration in dynamical astronomy”, App. Num. Math. 68 (2013) 58-72.
- [13] E. Gerlach, S. Eggl, Ch. Skokos, J. D. Bodyfelt and G. Papamikos, “High order three part split symplectic integration schemes”, 10th HSTAM International Congress on Mechanics, 2013.
- [14] E. Gerlach, J. Meichsner and Ch. Skokos, “On the symplectic integration of the discrete nonlinear Schrodinger equation with disorder”, Manuscript 2016.
- [15] Ch. Skokos and E. Gerlach, “Numerical integration of variational equations”, Phy. Rev. E **82**, 036704 (2010).
- [16] Ch. Skokos, I. Gkolias and S. Flach, “Nonequilibrium Chaos of Disordered Nonlinear Waves”, Phy. Rev. Lett., PRL **111**, 064101 (2013)
- [17] J. Billy et al, “Direct observation of Anderson localization of matter waves in a controlled disorder”, nature, vol 453, 2008
- [18] S. A. Chin, “Symplectic integrators from composite operator factorizations”, Phys. Lett. A 226 (1997) 344-348.
- [19] M. Suzuki, “Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations”, Phys. Lett. A, Vol. 146, no. 6 (1990).
- [20] R. I. McLachlan and G. R. W. Quispel, “Geometric integrators for ODEs”, J. Phys. A: Math. Gen. 39 (2006) 5251-5285
- [21] Ch. Skokos, D.O. Krimer, S. Komineas and S. Flach, “Delocalization of wave packets in disordered nonlinear chains”, Phys. Rev. E 79, 056211 (2009).
- [22] T. V. Lapyteva, J. D. Bodyfelt, D.O. Krimer, Ch. Skokos and S. Flach, “The crossover from strong to weak chaos for nonlinear waves in disordered systems”, EPL, 91 30001 (2010).